Parametrization of spin-1 classical states

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We give an explicit parametrization of the set of mixed quantum states and of the set of mixed classical states for a spin–1. Classical states are defined as states with a positive Glauber-Sudarshan P-function. They are at the same time the separable symmetric states of two qubits. We explore the geometry of this set, and show that its boundary consists of a two-parameter family of ellipsoids. The boundary does not contain any facets, but includes straight-lines corresponding to mixtures of pure classical states.

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I. INTRODUCTION

The rise of quantum information theory has led to a large interest in the geometry of specific sets of quantum states [1]. The most general quantum state of a quantum system with d-dimensional Hilbert space $\mathcal{H}$ is given by a density operator ρ that acts on $\mathcal{H}$. The density operator is a Hermitian, semi-definite positive operator with trace 1. Diagonalization shows immediately that it can always be written as a convex sum of projectors onto its eigenstates. The set $\mathcal{N}$ of all physical density operators is therefore the convex hull of projectors onto all pure states in $\mathcal{H}$. Certainly the most popular set of states in quantum information theory is the set of separable states, defined for a physical system that can be partitioned into at least two subsystems. If ρ can be written as a convex sum of tensor products of projectors onto pure states of the subsystems, that state is called "separable", and "entangled" otherwise [2]. Clearly, the set $\mathcal{S}$ of all separable states is a subset of $\mathcal{N}$. Knowing the geometry, and in particular the surface $\partial\mathcal{S}$ of the set $\mathcal{S}$, is an important but difficult problem, as it would allow to determine immediately whether a given state is inside or outside $\mathcal{S}$, or, in other words, whether it is entangled or not. In the case of two qubits, $\partial\mathcal{S}$ was shown to be smooth in the interior of $\mathcal{N}$ [3]. Furthermore, for a general bipartite state, it was shown that $\partial\mathcal{S}$ is not a polytope [4] and, using non-linear entanglement witnesses, that it does not contain any facets [5].

Recently we introduced the convex set $\mathcal{C} \subseteq \mathcal{N}$ of "classical states" of a spin (or angular momentum) with total angular momentum j [6]. It is defined as the convex hull of projectors onto coherent states of $SU(2)$, which have the physical interpretation of having minimal quantum uncertainty of the angular momentum vector, i.e. they resemble as much as possible a point in classical phase space. The interest of classical states is that they are defined even for a single spin, i.e. when the question of entanglement does not even arise. Furthermore, they allow a definition of what a genuinely "quantum" state might be. Indeed, one may define a measure of "quantumness" [7] of a spin state by measuring its distance from $\mathcal{C}$, just as the distance to $\mathcal{S}$ provides a measure of entanglement (see [8] for an overview of this type of entanglement measure). If distance from $\mathcal{C}$ is measured through the Bures distance [1, 9], quantumness of symmetric multi-qubit states becomes essentially equivalent to their geometrical entanglement [10]. Also note that the set of classical states of a spin–1 is identical to the set of separable symmetric states (under the exchange of particles) of two qubits.

States of a spin with maximal quantumness with given total angular momentum j (i.e. with Hilbert space dimension $2j+1$), the "Queens of Quantum", can always be found among pure states [7]. However, if $\partial\mathcal{C}$ contains facets, there might exist mixed states with the same maximal quantumness. Knowing the form of the surface of the set of classical states is therefore important. In [7] it was shown that for spin–1 states maximal quantumness is reached only for pure states, but for larger j maximally quantum states might comprise mixed states. After what was said above about how little is known about the surface $\partial\mathcal{S}$ of the set of separable states, one might expect that determining $\partial\mathcal{C}$ is a difficult problem as well. This is indeed the case, but nevertheless, here we give a complete characterization of $\partial\mathcal{C}$ for the case of a qutrit (i.e. a three state system, corresponding to a pseudo-angular momentum $j=1$). We show that in this case $\mathcal{C}$, as $\mathcal{S}$, is not a polytope either, but rather a continuous family of ellipsoids. We also show that the surface of $\mathcal{C}$ contains families of straight lines.

II. SPIN–$\frac{1}{2}$ CASE

Let us first consider the trivial case of a spin–$\frac{1}{2}$ system. In this case it was shown in [6] that the set $\mathcal{C}$ of classical states coincides with $\mathcal{N}$. Any 2×2 density matrix can be expanded over the basis of Pauli matrices σ_a as

$$\rho = \frac{1}{2}\mathbf{1}_2 + \sum_a u_a\sigma_a \tag{1}$$

with $\mathbf{1}_2$ the 2×2 identity matrix and u_a are real numbers with $a = x, y, z$. The matrix ρ given by (1) is Hermitian and has trace 1, therefore it belongs to $\mathcal{N}$ if and only if it is positive. The characteristic polynomial of ρ can be put under the form

$$\det\left(x\mathbf{1}_2 - \rho\right) = x^2 - x + \frac{1 - \sum_a u_a^2}{4}. \tag{2}$$

Its roots are positive if and only if

$$\sum_a u_a^2 \leq 1. \tag{3}$$

Equation (3) is thus the necessary and sufficient condition for $\rho \in \mathcal{N}$ in terms of the coordinates u_a which parametrize ρ. The boundary $\partial\mathcal{N}$ of $\mathcal{N}$ corresponds to points where one of the eigenvalues of ρ vanishes. In terms of coordinates u_a it is given by the equation $\sum_a u_a^2 = 1$. The parametrization of $\partial\mathcal{N}$ is the parametrization of a sphere.

The results above correspond to the usual picture of the Bloch sphere for spin–$\frac{1}{2}$. The vector $\mathbf{u}$ is the Bloch vector, and the boundary of (classical) states is the boundary of the sphere, corresponding to rank-one matrices, or pure states, with Bloch vector of length 1. Such a simple picture does not exist for higher spins. Let us now consider the case of spin–1 states.

III. CLASSICALITY CRITERION FOR SPIN–1 STATES

We start with the expansion of a mixed spin–1 state over the basis formed by the 3×3 angular momentum matrices, J_a, $a = x, y, z$, together with the $(J_aJ_b + J_bJ_a)/2$ and the 3×3 identity matrix $\mathbf{1}_3$. We define a vector $\mathbf{u}$ and a matrix W through coefficients of this expansion, as

$$\rho = \frac{1}{3}\mathbf{1}_3 + \frac{1}{2}\mathbf{u}.\mathbf{J} + \frac{1}{2}\sum_{a,b=x,y,z}\left(W_{ab} - \frac{1}{3}\delta_{ab}\right)\frac{J_aJ_b + J_bJ_a}{2}. \tag{4}$$

The coefficients $\mathbf{u}$ and W are related with ρ through

$$u_a = \mathrm{tr}\left(\rho J_a\right), \quad W_{ab} = \mathrm{tr}\rho\left(J_aJ_b + J_bJ_a\right) - \delta_{ab}. \tag{5}$$

Note that $\mathbf{u}$ is real and that W is a real symmetric matrix, with tr $W = 1$.

The expression (4) ensures that ρ is Hermitian with $\mathrm{tr}\rho = 1$. Thus the set $\mathcal{N}$ of density matrices is the set of matrices of the form (4) with $\rho \geq 0$. According to [6], ρ is a density matrix associated with a classical state if and only if the real symmetric 3×3 matrix Z with matrix elements

$$Z_{ab} = W_{ab} - u_a u_b \tag{6}$$

is non-negative, thus the set $\mathcal{C}$ of classical density matrices is the set of matrices of the form (4) with $Z \geq 0$.

IV. SET $\mathcal{N}$ OF DENSITY MATRICES

The class of density matrices $\mathcal{N}$ comprises Hermitian non-negative matrices with trace 1. Its parametrization is important in many applications and can be achieved in several ways. One of these is based on the representation $\rho = U\ \mathrm{diag}[\lambda_1..\lambda_{2j+1}]\ U^{-1}$, $\lambda_i \geq 0$, $\sum \lambda_i = 1$, where U runs over a subset of the unitary group chosen such that each ρ is obtained once and only once. A parametrization for the case $j = 1$ using Gell-Mann matrices is considered in [11]; see also [12] for the closely related problem of 3×3 coherence matrices of nonparaxial light. Another method uses the factorization $\rho = VV^\dagger$ where V is upper triangular [13]. Here we shall give an alternative representation based on the formula (4).

Parameters $\mathbf{u}$ and W have the nice feature, similar to the Bloch picture in the two-dimensional case, that under rotation of the coordinate system with an orthogonal rotation matrix O, ρ is transformed into a matrix with parameters $O\mathbf{u}$ and OWO^T, i.e. $\mathbf{u}$ and W transform with the same rotation O. Thus it will be convenient to express them in a basis where W is diagonal, $W = \mathrm{diag}[\mu_x, \mu_y, \mu_z]$; we shall write the result as

$$\rho = \rho' + \frac{1}{2}\mathbf{u}.\mathbf{J},$$
$$\rho' = \frac{1}{2}\left(\mu_x J_x^2 + \mu_y J_y^2 + \mu_z J_z^2\right). \tag{7}$$

Considering that tr $W = 1$ and that, in a state ρ with angular momentum 1, we have $0 \leq \mathrm{tr}\ \rho J_a^2 \leq 1$, $0 \leq |\mathrm{tr}\rho\mathbf{J}| \leq 1$ we obtain the necessary conditions on the parameters in (7),

$$\sum_{a=x,y,z} \mu_a = 1,$$
$$-1 \leq \mu_a \leq 1, \quad a = x, y, z, \tag{8}$$
$$u_x^2 + u_u^2 + u_z^2 \leq 1. \tag{9}$$

For the "truncated" matrix $\rho' = \rho|_{\mathbf{u}=0}$ conditions (8) are also sufficient to guarantee that $\rho' \in \mathcal{N}$. Indeed, direct calculation shows that the eigenvalues of ρ' are

$$\lambda'_a = \frac{1 - \mu_a}{2} \geq 0, \quad a = x, y, z, \tag{10}$$

while the corresponding eigenvectors $|v_a\rangle$ are eigenvectors of J_a with eigenvalue zero. Since $\langle v_a|\mathbf{J}|v_a\rangle = \mathbf{0}$, we have $\langle v_a|\rho|v_a\rangle = \lambda'_a$. These averages give an upper bound to the smallest eigenvalue of ρ. It immediately follows that if ρ belongs to $\mathcal{N}$ then so does ρ' but not vice versa.

In fact, a stronger statement can be made. Let $\rho_\kappa = \rho' + \frac{\kappa}{2}\mathbf{u}.\mathbf{J}$ be a density matrix differing from ρ by a positive factor κ in the part linear in $\mathbf{J}$. Then the lowest eigenvalue of ρ_κ is a monotonically decreasing function of κ. Consequently if ρ_κ with some $\kappa = \kappa_1$ belongs to $\mathcal{N}$ then so do all matrices with $0 \leq \kappa < \kappa_1$. These assertions follow from the following theorem of perturbation theory (for a proof, see the Appendix): Let $H = H_0 + \kappa V$, $\kappa \geq 0$,

be a Hermitian matrix whose spectrum is bounded from below, and $E_0(\kappa), \psi_0(\kappa)$ be its lowest eigenvalue and eigenstate. Suppose that $E_0(0)$ is non-degenerate and $\langle\psi_0(0)|V|\psi_0(0)\rangle = 0$. Then $E_0(\kappa)$ is a monotonically decreasing function. Setting $H_0 \to \rho'$, $V \to (1/2)\mathbf{u}.\mathbf{J}$ we come to the statement above.

Let us find the constraints sufficient and necessary to guarantee non-negativity of ρ. The characteristic polynomial of ρ written in the form (4) can be presented as

$$\det(x\mathbf{1}_3 - \rho) = x^3 - x^2 + ax - \det\rho \tag{11}$$

with

$$a = \frac{1}{4}\left(-|\mathbf{u}|^2 + 1 - \frac{\mathrm{tr}W^2 - 1}{2}\right). \tag{12}$$

Since ρ is Hermitian the three roots of the polynomial are real. According to Descartes' rule of signs, a polynomial of the form $x^3 - x^2 + ax - b$ with three real roots has all its roots positive if and only if a and b are positive. Thus $\rho \in \mathcal{N}$ iff $\det\rho \geq 0$ and

$$1 - |\mathbf{u}|^2 + \frac{1 - \mathrm{tr}W^2}{2} \geq 0. \tag{13}$$

The latter condition defines a sphere in the u-space. Since it does not depend on the basis in which $\mathbf{u}$ and W is expressed, we can write Eq. (13) in the basis where W is diagonal; in that basis it becomes

$$|\mathbf{u}|^2 \leq 1 + \mu_x\mu_y + \mu_x\mu_z + \mu_y\mu_z. \tag{14}$$

One can check that the condition $\det\rho \geq 0$ can be rewritten

$$\langle\mathbf{u}|W|\mathbf{u}\rangle - |\mathbf{u}|^2 + \frac{1 - \mathrm{tr}W^2}{2} - \det W \geq 0, \tag{15}$$

which in the basis where W is diagonal becomes

$$\sum_a u_a^2(1 - \mu_a) \leq (1 - \mu_x)(1 - \mu_y)(1 - \mu_z). \tag{16}$$

When all μ_a differ from 1, it defines an ellipsoid in the $u-$space lying inside both spheres (9) and (14). Indeed, the squared radius of the ellipsoid along the x-axis for instance is given by

$$r_x^2 = (1 - \mu_y)(1 - \mu_z) = \mu_x + \mu_y\mu_z \tag{17}$$

and using the fact that $1 - \mu_x^2 \geq 0$ we get

$$r_x^2 \leq 1 - \mu_x^2 + r_x^2 = 1 + \mu_x\mu_y + \mu_x\mu_z + \mu_y\mu_z. \tag{18}$$

On the other hand, the inequality $\mu_y \geq -\mu_z$ (coming from $\mu_x \leq 1$) yields

$$r_x^2 = (1 - \mu_y)(1 - \mu_z) \leq 1 - \mu_z^2 \leq 1, \tag{19}$$

thus the ellipsoid also lies within the sphere of radius 1. However, when one or two μ_a are equal to 1, then Eqs. (9) and (14) have to be taken into account. We finally obtain that $\rho \in \mathcal{N}$ if and only if the (u_a, μ_a) verify one of the following conditions:

1. All μ_a are such that $-1 \leq \mu_a < 1$, and
$$\sum_a \frac{u_a^2}{\mu_a + \mu_b\mu_c} \leq 1, \tag{20}$$
with $\sum_a \mu_a = 1$ and b, c are the two indices which differ from a (this automatically implies (9),(14));

2. Exactly one μ_a is equal to 1, say $\mu_z = 1$. Then $\mu_y = -\mu_x$ with $-1 < \mu_x < 1$, and $u_x = u_y = 0$. Equation (14) yields $u_z^2 \leq 1 - \mu_x^2$ and is obviously more restrictive than (9);

3. Two of the μ_a are equal to 1, say $\mu_y = \mu_z = 1$, then $\mu_x = -1$, $u_x = u_y = u_z = 0$. This corresponds, up to rotation, to the state $|1,0\rangle\langle 1,0|$ (in $|j,m\rangle$ notation).

The boundary $\partial\mathcal{N}$ of $\mathcal{N}$ corresponds to points where one of the inequalities (13) or (15) becomes an equality. For $\mu_a \neq 1$ (case 1 above), Eq. (15), equivalent to the equation of the ellipsoid (16), is more restrictive than (13) so that $\partial\mathcal{N}$ coincides with the surface of the ellipsoid (20). The cases when one or two μ_a are equal to 1 correspond to cases 2 and 3, where equality is reached in (16). Therefore, the surface $\partial\mathcal{N}$ is the union of points corresponding to case 1 when (20) is an equality, and of points corresponding to cases 2 and 3.

Points of $\partial\mathcal{N}$ corresponding to case 1, with equality in (20), belong to a two-parameter set of ellipsoids that can be parametrized by $\mu_a \in [-1, 1[$ and

$$\mathbf{u} = \begin{pmatrix} \sqrt{\mu_x + \mu_y\mu_z}\cos\theta\cos\varphi \\ \sqrt{\mu_y + \mu_x\mu_z}\cos\theta\sin\varphi \\ \sqrt{\mu_z + \mu_x\mu_y}\sin\theta \end{pmatrix}, \quad \theta \in [0, \pi], \ \ \varphi \in [0, 2\pi[. \tag{21}$$

Any density matrix $\rho \in \mathcal{N}$ for spin 1 is parametrized by 8 real numbers. Thus $\partial\mathcal{N}$ should be parametrized by 7 numbers. For points corresponding to case 1, besides μ_1, μ_2, θ and φ, the three remaining parameters correspond to the three angles that parametrize the orthogonal matrix required to diagonalize W. These orthogonal transformations also include transpositions of axes x, y, z; to get each matrix once and only once we must introduce restrictions on μ_a, say, $\mu_z \leq \mu_y \leq \mu_x$. One way to do so is to use the eigenvalues λ'_a of ρ' as auxiliary variables, with $\mu_a = 1 - 2\lambda'_a$, setting

$$\begin{pmatrix} \lambda'_x \\ \lambda'_y \\ \lambda'_z \end{pmatrix} = \begin{pmatrix} \sin^2\theta'\sin^2\varphi' \\ \sin^2\theta'\cos^2\varphi' \\ \cos^2\theta' \end{pmatrix} \tag{22}$$

with $\theta' \in]0, \arctan(1/\cos(\varphi'))]$ and $\varphi' \in]0, \pi/4]$. Points of $\partial\mathcal{N}$ corresponding to cases 2 and 3 are of measure zero on the surface.

V. SET $\mathcal{C}$ OF CLASSICAL STATE DENSITY MATRICES

We now characterize the set $\mathcal{C}$ of classical states. A necessary and sufficient condition for classicality of a state

$\rho \in \mathcal{N}$ is $Z \geq 0$, where Z is given by Eq. (6). The characteristic polynomial of Z reads

$$\det(x\mathbf{1}_3 - Z) = x^3 - \mathrm{tr}Zx^2 + \frac{(\mathrm{tr}Z)^2 - \mathrm{tr}Z^2}{2}x - \det Z. \tag{23}$$

Since Z is real symmetric the three roots of the characteristic polynomial are real. As in the previous section, Descartes' rule of signs implies that the roots are positive, i.e. ρ is a density matrix associated with a classical state, if and only if the three conditions

$$\mathrm{tr}Z \geq 0,\ (\mathrm{tr}Z)^2 \geq \mathrm{tr}Z^2 \text{ and } \det Z \geq 0 \tag{24}$$

are fulfilled. In terms of $\mathbf{u}$ and W one has

$$\begin{aligned} \mathrm{tr}Z &= 1 - |\mathbf{u}|^2 && (25)\\ \mathrm{tr}Z^2 &= \mathrm{tr}W^2 - 2\langle\mathbf{u}|W|\mathbf{u}\rangle + |\mathbf{u}|^4 && (26)\\ \det Z &= \det(W - |\mathbf{u}\rangle\langle\mathbf{u}|)\,. && (27) \end{aligned}$$

Using (9) and (25) we see that condition $\mathrm{tr}Z \geq 0$ is fulfilled by any density matrix. The two remaining conditions on Z do not depend on the basis in which $\mathbf{u}$ and W is expressed, thus we can write them in the basis where W is diagonal with eigenvalues μ_x, μ_y, μ_z. Using Eqs. (25)–(26), condition $(\mathrm{tr}Z)^2 \geq \mathrm{tr}Z^2$ is equivalent to

$$\sum_a u_a^2(1-\mu_a) \leq \mu_x\mu_y + \mu_x\mu_z + \mu_y\mu_z. \tag{28}$$

Condition $\det Z \geq 0$ becomes

$$\mu_y\mu_z u_x^2 + \mu_x\mu_z u_y^2 + \mu_x\mu_y u_z^2 \leq \mu_x\mu_y\mu_z. \tag{29}$$

A state ρ belongs to $\mathcal{C}$ if and only if it verifies Eqs. (8)–(9) and (28)–(29). A necessary condition for Z to be positive is that its diagonal elements $\mu_a - u_a^2$ are positive, which entails positivity of the μ_a and thus $\mu_a \in [0,1]$. If all μ_a differ from 0 and 1 then (28) and (29) describe ellipsoids in u-space, with axes lengths respectively given by r_a and r'_a with

$$r_a^2 = \frac{\mu_x\mu_y + \mu_x\mu_z + \mu_y\mu_z}{1-\mu_a}, \qquad {r'_a}^2 = \mu_a \tag{30}$$

Since all $\mu_a \in]0,1[$, one has $r_a > r'_a$, thus (29) is more restrictive than (28). It is also more restrictive than the equation of the sphere Eq. (9) since $r'_a < 1$. If $\mu_a = 0$ or $\mu_a = 1$ for at least one value of a, one has to consider all equations again. Finally $\rho \in \mathcal{C}$ if and only if the parameters μ_a and u_a correspond to the following situations:

1. All $\mu_a \in]0,1[$ and

$$\frac{u_x^2}{\mu_x} + \frac{u_y^2}{\mu_y} + \frac{u_z^2}{\mu_z} \leq 1, \tag{31}$$

   that is, $\mathbf{u}$ corresponds to a point inside an ellipsoid centered at $(0,0,0)$ with half-axes of length $\sqrt{\mu_a}$;

2. Exactly one of the μ_a is equal to 0, say $\mu_z = 0$. Then from (29) one must have $u_z = 0$ and from (28)

$$\frac{u_x^2}{\mu_x} + \frac{u_y^2}{\mu_y} \leq 1. \tag{32}$$

   This corresponds to the situation above flattened to 2 dimensions;

3. Two μ_a are zero, e. g. $\mu_y = \mu_z = 0$. Then $\mu_x = 1$ and from (28) one must have $u_y = u_z = 0$, which leaves the condition $|u_z| \leq 1$. Again this corresponds to the situation (31), flattened to 1 dimension.

A point ρ belongs to the boundary $\partial\mathcal{C}$ of $\mathcal{C}$ if one of the inequalities (24) becomes an equality. States with one or two μ_a equal to 0 always verify $\det Z = 0$ and thus lie on the boundary $\partial\mathcal{C}$. When all μ_a are in $]0,1[$, the condition that $\det Z = 0$ is equivalent to equality in (31), which corresponds to points u_a which lie on the surface of the ellipsoid (31). Condition $\mathrm{tr}Z = 0$ is equivalent to equality in (9), while condition $(\mathrm{tr}Z)^2 = \mathrm{tr}Z^2$ is equivalent to equality in (28). Since the ellipsoid (31) lies inside both the sphere (9) and the ellipsoid (28), the points corresponding to either of these cases must lie on the surface of the ellipsoid (31). Therefore, points on the boundary $\partial\mathcal{C}$ correspond to case 1 above when (31) becomes an equality, or to cases 2 or 3.

In the main case (equality in (31)) the surface is a two-parameter set of ellipsoids that can be parametrized by $\mu_a \in]0,1[$ with $\sum_a \mu_a = 1$, e. g.,

$$\boldsymbol{\mu} = \begin{pmatrix} \sin^2\theta_1 \sin^2\varphi_1 \\ \sin^2\theta_1\cos^2\varphi_1 \\ \cos^2\theta_1 \end{pmatrix}, \tag{33}$$

and

$$\mathbf{u} = \begin{pmatrix} \sin\theta_1\sin\varphi_1\cos\theta_2\cos\varphi_2 \\ \sin\theta_1\cos\varphi_1\cos\theta_2\sin\varphi_2 \\ \cos\theta_1\sin\theta_2. \end{pmatrix} \tag{34}$$

Again, the parametrization requires three more angles to take into account the orthogonal matrix required to diagonalize W. If α, β and γ are the three Euler angles that parametrize the orthogonal matrix O then one has the complete parametrization

$$\begin{aligned} \mathbf{u} &= O(\alpha,\beta,\gamma)\begin{pmatrix} \sin\theta_1\sin\varphi_1\cos\theta_2\cos\varphi_2 \\ \sin\theta_1\cos\varphi_1\cos\theta_2\sin\varphi_2 \\ \cos\theta_1\sin\theta_2 \end{pmatrix}, && (35)\\ W &= O\begin{pmatrix} \sin^2\theta_1\sin^2\varphi_1 & & 0 \\ & \sin^2\theta_1\cos^2\varphi_1 & \\ 0 & & \cos^2\theta_1 \end{pmatrix} O^T \end{aligned}$$

with $O = O(\alpha,\beta,\gamma)$. To summarize, the number of essential parameters for the set $\mathcal{C}$ (excluding rotations of

the coordinate system) is 5, and for the surface $\partial\mathcal{C}$ it is 4.

In order to obtain each classical matrix ρ once and only once we shall demand that $\mu_x \leq \mu_y \leq \mu_z$ which means that the range in (33)–(35) has to be restricted to $\theta_1 \in]0, \arctan(1/\cos(\varphi_1))]$ and $\varphi_1 \in]0, \pi/4]$ (see [11]).

VI. SOME EXAMPLES

We first give an example of a non-classical state. In section IV we saw that the case $\mu_y = \mu_z = 1$ corresponds to state $\rho = |1,0\rangle\langle 1,0|$. According to [7] this is the most quantum spin–1 state. Its Majorana representation corresponds to two points diametrically opposed on the Bloch sphere, e.g. north and south pole.

Let us now consider the case where two of the μ_a vanish (case 3 of the above section), say, $\mu_y = \mu_z = 0$. Then $\mu_x = 1$ and Eq. (20) implies that $u_y = u_z = 0$. Then $\rho \in \mathcal{C}$ if and only if $u_x = u \in [-1, 1]$. In this case the ellipsoid is flattened to a line. The state ρ can be decomposed as

$$\rho = \frac{1-u}{2}|\psi^{(-)}\rangle\langle\psi^{(-)}| + \frac{1+u}{2}|\psi^{(+)}\rangle\langle\psi^{(+)}|, \tag{36}$$

with

$$|\psi^{(\pm)}\rangle = \frac{|1,-1\rangle \pm \sqrt{2}|1,0\rangle + |1,1\rangle}{2}. \tag{37}$$

The pure states $|\psi^{(\pm)}\rangle$ are eigenvectors of J_x corresponding to the eigenvalues ± 1, i. e., they are coherent states directed along or opposite to the x-axis. Since $u \in [-1, 1]$, ρ is a classical mixture of two coherent states. It forms a one-parameter family of classical states. Since the entire family is inside $\partial\mathcal{C}$, this represents a one-dimensional line on the surface. This indicates that the surface $\partial\mathcal{C}$ is not necessarily strictly convex. Nevertheless, we now show that the surface $\partial\mathcal{C}$ does not contain facets, that is, the surface is not locally a (7-dimensional) hyperplane.

For a state $\rho \in \mathcal{N}$ and a three-dimensional real vector $\mathbf{t}$ with $|\mathbf{t}| = 1$, we define

$$Q_{\mathbf{t}} = 2\langle J_{\mathbf{t}}^2\rangle - \langle J_{\mathbf{t}}\rangle^2 - 1. \tag{38}$$

As noted in [6], the classicality criterion $Z \geq 0$ is equivalent to $Q_{\mathbf{t}} \geq 0$ for all $\mathbf{t}$. For fixed $\mathbf{t}$, $Q_{\mathbf{t}} = 0$ defines a quadric surface $S_{\mathbf{t}}$ in the eight-dimensional space of variables $\{u_a, W_{ab}\}$. Its equation can be rewritten as $Q_{\mathbf{t}} = \sum_{a,b}(W_{ab} - u_a u_b)t_a t_b = 0$, with t_a, $a = x, y, z$, fixed. Each surface $S_{\mathbf{t}}$ separates the space of all states $\mathcal{N}$ into two subsets. The subset of states with $Q_{\mathbf{t}} < 0$ contains only genuinely quantum states, as they violate the condition $Q_{\mathbf{t}} \geq 0$ for at least one $\mathbf{t}$. The subset of states with $Q_{\mathbf{t}} > 0$ is convex: indeed, a linear change of variables with a new variable $X_1 = \sum_a u_a t_a$ yields $Q_{\mathbf{t}} = X_1^2 +$ linear terms. Now let M be a point on $\partial\mathcal{C}$ and suppose there exists a sphere B_ϵ with radius ϵ, centered on M, such that inside B_ϵ the surface $\partial\mathcal{C}$ is a piece of a hyperplane (see Fig. 1). By definition of $\mathcal{C}$, the sphere is split into two equal halves, one containing only quantum states and the other one containing only classical states. But since $S_{\mathbf{t}}$ is not a flat surface, part of the states in the latter half-sphere must lie on the subset on states with $Q_{\mathbf{t}} < 0$ (see Fig. 1), which entails a contradiction.

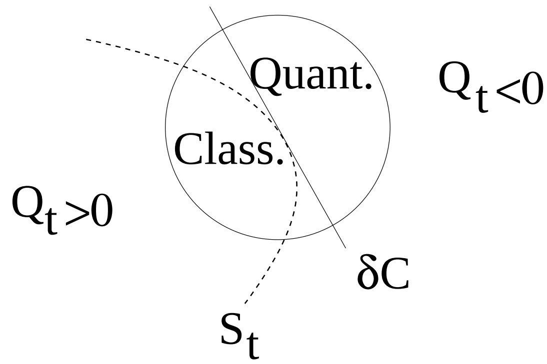

FIG. 1: Local geometry at a point on the surface $\partial\mathcal{C}$ of the set of classical states.

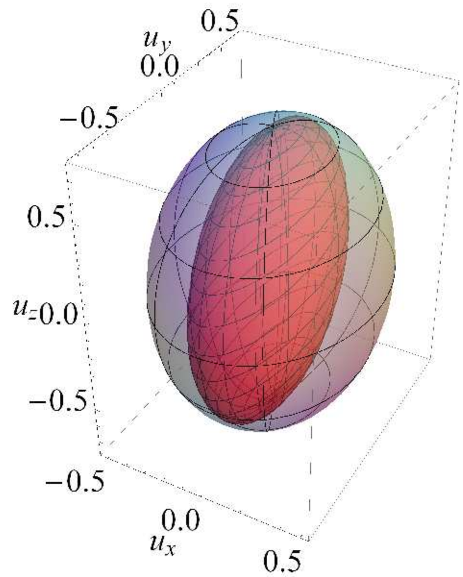

FIG. 2: (Color online) Boundaries $\partial\mathcal{N}$ of the set of physical density matrices (outer ellipsoid) and $\partial\mathcal{C}$ of the classical states (inner ellipsoid) for $\mu_x = 0.05$, $\mu_y = 0.4$, and $\mu_z = 0.55$ in terms of the dimensionless components u_i of the vector $\mathbf{u}$ defined in eq.(4). The two ellipsoids do not touch in general, and their axes coincide.

Another interesting example is the thermal state

$$\rho = e^{-\beta H}/\mathrm{tr} e^{-\beta H} \tag{39}$$

of a system with Hamiltonian $H = J_z^2$ and inverse temperature $\beta = 1/k_B T$, with k_B Boltzmann's constant. For temperature $T = 0$, the thermal state is the ground state $|1,0\rangle$, which is the most quantum state possible. For $T \to \infty$ on the other hand, ρ approaches the identity

matrix and is therefore classical. The transition temperature to classicality can be found exactly from the boundary $\partial\mathcal{C}$. The parametrization of (39) gives $\mathbf{u}=\mathbf{0}$ and

$$W=\begin{pmatrix} \frac{e^\beta}{2+e^\beta} & 0 & 0 \\ 0 & \frac{e^\beta}{2+e^\beta} & 0 \\ 0 & 0 & \frac{2-e^\beta}{2+e^\beta} \end{pmatrix}. \tag{40}$$

The inequality in (31) is always satisfied. The condition that $\mu_a \in [0,1]$ reduces to $0 \le e^\beta \le 2$. Therefore, ρ is classical if and only if $\beta \le \ln 2$.

As a last example, consider a state with $\mu_x = 0.05$, $\mu_y = 0.4$, and $\mu_z = 0.55$. One can then specify the boundaries $\partial\mathcal{C}$ and $\partial\mathcal{N}$ solely in terms of the u_a. Fig.2 shows that $\partial\mathcal{C}$ is indeed an ellipsoid inside the ellipsoid given by $\partial\mathcal{N}$.

VII. CONCLUSIONS

To summarize, we have found an explicit representation of the set $\mathcal{C}$ of classical spin–1 states, Eq. (31) defined as the convex hull of spin–1 SU(2) coherent states. The set $\mathcal{C}$ consists of a family of ellipsoids. The surface of the set contains straight lines, thus this allows the existence of linear families of genuinely quantum states with exactly the same quantumness. Our results allow to visualize the set of classical states and to determine analytically under what conditions a density matrix that depends on one or several parameters becomes genuinely "quantum".

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Appendix

Let $E_0(\kappa)$ be the lowest eigenvalue of the parameter-dependent Hermitian matrix $H(\kappa)$ and ψ_0 its corresponding eigenvector. At values of κ such that the ground level is non-degenerate the second derivative of $E_0(\kappa)$ is non-positive. This follows, e.g., from the identity $E_0'' = -2\langle\psi_0|T_0|\psi_0\rangle$ with T_0 denoting a manifestly positive operator,

$$T_0 = \frac{\partial H}{\partial\kappa} Q_0 \left(H - E_0\right)^{-1} Q_0 \frac{\partial H}{\partial\kappa}, \qquad Q_0 = \hat{1} - |\psi_0\rangle\langle\psi_0|\,. \tag{41}$$

Assume now that at $\kappa = 0$ the ground state is non-degenerate and besides, the first derivative $E_0'(0) = 0$. Then for all positive κ the ground state energy will be monotonically decreasing (or at best non-growing) function of κ. Indeed, if we first assume that $E_0(\kappa)$ is not degenerate for all $k \ge 0$ then we have $E_0'(\kappa) = \int_0^\kappa E_0''(x)dx \le 0$ for $\kappa \ge 0$. The result remains true even if there is level crossing at some $\kappa = \kappa_1$ since then for $\kappa > \kappa_1$ we can write $E_0'(\kappa) = E_0'(\kappa_1 + 0^+) + \int_{\kappa_1+0^+}^\kappa E_0''(x)dx$. The integral is negative from the same argument as above, and $E_0'(\kappa_1+0^+)$ is the slope immediately after the crossing, which must be smaller than the slope immediately before the crossing, which we know to be negative.

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